Hydrogen-Induced Metal-Insulator Transition in Yttrium

Probing the Local Electronic Structure with Soft X-Ray Emission and Absorption

Yttrium metal becomes an optically transparent insulator when loaded with hydrogen. Although this metal-insulator transition is conceptually simple, the changes in the electronic structure that cause it are not fully understood. A Swedish group working at the ALS is using x-ray emission and absorption to attack the problem. Their measurements have confirmed the emergence of a band gap characteristic of a transparent insulator with increasing hydrogen content. The measurements also provide clues about the influence of hydrogen on yttrium core electronic states, a question of great interest, since it is generally anticipated that there are many other possibilities of tuning material properties in this way

Soft x-ray emission spectroscopy (SXES) allows direct probing of the local valence electronic structure in terms of the symmetry-selected *occupied* density of states, whereas soft x-ray absorption spectroscopy (SXAS) allows one to probe the *unoccupied* density of states. The combination of SXES and SXAS thus provides a means to study metal–insulator transitions. Moreover, the substantial attenuation length of soft x rays allows SXES to be applied to buried structures or to samples at ambient gas pressures. This capability is necessary for studies of hydrogen loading, since samples have to be either capped after hydrogen loading or exposed to hydrogen gas during measurement.

In experiments at Beamline 7.0 of the ALS, the yttrium $M_{4,5}$ emission spectra (transitions to $3d_{3/2}$ and $3d_{5/2}$ core states) were recorded with the Uppsala University SXES spectrometer installed at this beamline. The soft x-ray absorption spectra were recorded in fluorescence-yield mode with the same instrument. The data were obtained for samples that were hydrogen loaded and capped in the preparation process. Three samples of different hydrogen loading were studied: yttrium metal (no loading), yttrium dihydride, and yttrium trihydride.

Among the SXES spectra for valence → 3d core transitions in the three samples along with the corresponding SXAS spectra, for yttrium metal there is a sharp edge at the top of the valence band identified as the Fermi level. SXAS shows an onset at this energy, which implies an overlap between the top of the valence band and the bottom of the conduction band. The overlap reflects the metallic character of yttrium. A substantial change is observed in the x-ray emission with increasing hydrogen content. The total intensity increases, and a strong hybridization feature appears at about 6 eV to 7 eV below the Fermi level. At the Fermi level, one still observes features of reduced intensity. In the trihydride spectrum, a further reduction in intensity is observed at the Fermi level, indicating a band gap with an estimated width of 2.5 eV. This observation is consistent with the reported transparency and slightly yellowish color of yttrium trihydride.

In the emission spectra for yttrium $4p_{3/2} \rightarrow 3d_{5/2}$ core-core transitions in the same three samples, one observes increased bandwidth for the hydrides and a shift to lower transition energy. In a simple picture, one expects the inner, more localized state in the hydrides to be more affected by a change in charge density, so the energy shift suggests that the hydrogen uptake leads to electron *donation* to the yttrium sites. However, first principles calculations of the electronic structure suggest a modified picture, in which instead of electron charge transfer, a strong hybridization between the hydrogen 1s states and the yttrium states occurs. The hybridization causes shifts similar to what one would expect from a charge-transfer model.

Joseph Nordgren (46-18-471-3554, joseph@fysik.uu.se), Department of Physics, Uppsala University, Box 530, S-751 21, Uppsala, SWEDEN.

B. Hjörvarsson J.-H. Guo, G. Andersson, R. C. C. Ward, R. Ahuja, O.Eriksson, M.R.Wells, C.Såthe, A. Agui, S. M. Butorin, and J. Nordgren, "Probing the local electronic structure in the H induced metal-insulator transition of Y." Submitted to *Phys. Rev. Lett.*

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HYDROGEN-INDUCED METAL-INSULATOR TRANSITION IN YTTRIUM

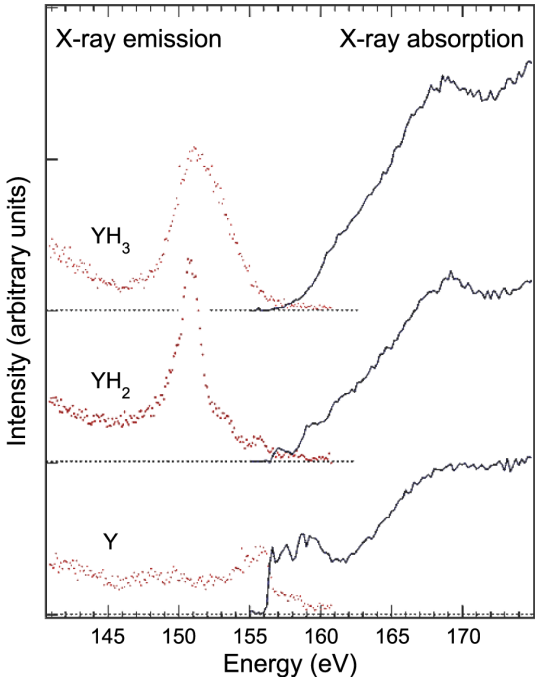
Probing the Local Electronic Structure with Soft X-Ray Emission and Absorption

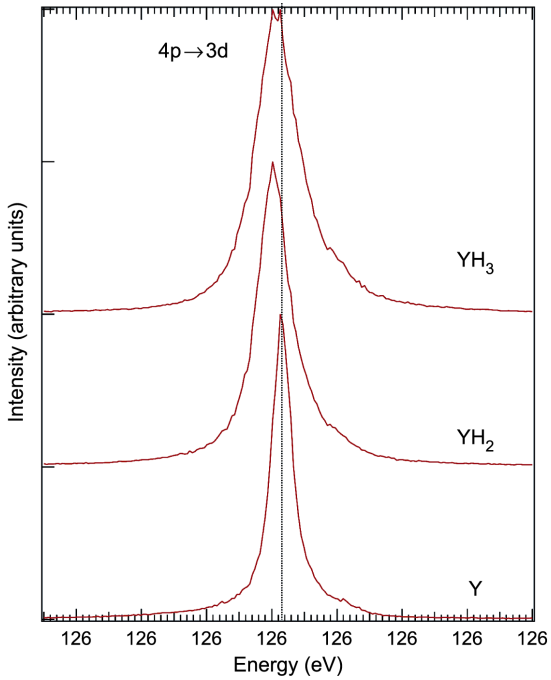
- **Hydrogen loading of Yttrium**
  - *Turns metal into optically transparent insulator (YH_3)*
  - *Electronic structure of transition not understood*
  - *Other opportunities for tuning properties of materials in a similar way*
- **Combined x-ray emission and fluorescence-yield absorption spectroscopy**
  - *Probes both occupied and unoccupied states → study metal-insulator transition*
  - *Applicable to buried interfaces and sample in gas environments → study hydrogen in metals*
- **Three samples with increasing hydrogen: Y, YH_2, and YH_3**
  - *Appearance of 2.5-eV band gap with hydrogen loading → transparent insulator*
  - *Observation of hybridization between yttrium 3d states and hydrogen*
  - *Peak shift and broadening for 4p → 3d core transition*

B. Hjörvarsson (Royal Institute of Technology, Sweden); J.-H. Guo, G. Andersson, R. Ahuja, O. Eriksson, C. Såthe, A. Agui, S.M. Butorin, and J. Nordgren (Uppsala University, Sweden); and R.C.C. Ward (University of Oxford, UK). [*J. Phys.: Condensed Matter* **11**, 199 (1999)].

HYDROGEN-INDUCED METAL-INSULATOR TRANSITION IN YTTRIUM

Probing the Local Electronic Structure with Soft X-Ray Emission and Absorption





X-ray emission (red) and absorption (black) spectra demonstrate the emergence of a band gap with increasing hydrogen content.

Emission spectra of core-core transitions in the same samples show an energy shift that suggests electron charge donation from hydrogen.

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